

Spin and chiral orderings of frustrated quantum spin chains

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Ordering of frustrated $S=1/2$ and 1 XY and Heisenberg spin chains with the competing nearest- and next-nearest-neighbor antiferromagnetic couplings is studied by exact diagonalization and density-matrix renormalization-group methods. It is found that the $S=1$ XY chain exhibits both gapless and gapped ‘chiral’ phases characterized by the spontaneous breaking of parity, in which the long-range order parameter is a chirality, $\kappa_i = S_i^x S_{i+1}^y - S_i^y S_{i+1}^x$, whereas the spin correlation decays either algebraically or exponentially. Such chiral phases are not realized in the $S=1/2$ XY chain nor in the Heisenberg chains.

Ordering of frustrated quantum spin chains has attracted considerable interest since these systems exhibit a rich variety of magnetic phases due to the interplay between quantum effect and frustration. We consider here an anisotropic frustrated quantum spin chain described by the XXZ Hamiltonian,

$$\mathcal{H} = \sum_{\rho=1}^2 \left\{ J_{\rho} \sum_{\ell} (S_{\ell}^x S_{\ell+\rho}^x + S_{\ell}^y S_{\ell+\rho}^y + \lambda S_{\ell}^z S_{\ell+\rho}^z) \right\}, \quad (1)$$

where \mathbf{S}_{ℓ} is the spin- S spin operator at the ℓ th site, $J_{\rho} > 0$ is the antiferromagnetic interaction between the nearest-neighbor ($\rho=1$) and the next-nearest-neighbor ($\rho=2$) spin pairs, and λ ($0 \leq \lambda \leq 1$) represents an exchange anisotropy. Note that $\lambda=0$ and $\lambda=1$ correspond to the XY and Heisenberg chains, respectively.

The ground state phase diagram of the corresponding $S=1/2$ system has been extensively studied either numerically [1,2] or analytically [3,4]. These studies have revealed that when J_2 is smaller than a critical value, *i.e.*, $j \equiv J_2/J_1 \leq j_c$, the system is in the gapless spin-fluid phase in which the antiferromagnetic spin correlation decays algebraically. By contrast, for larger values of $j > j_c$, the system is in the dimer phase with a finite energy gap above the doubly degenerate ground states. The dimer phase is characterized by the spontaneously breaking of both parity and translation symmetries with preserving time-reversal symmetry. The value of j_c has been estimated to be $j_c \cong 0.241$ for the Heisenberg chain [2]. Although there is no magnetic long-range order (LRO), the nature of the magnetic short-range order (SRO) changes at the Lifshitz point j_L , where $j_L \cong 0.5$ for the Heisenberg chain [1]. For $j \leq j_L$, the system has the standard Néel-type antiferromagnetic SRO and the structure factor $S(q)$ has a maximum at $q = \pi$, while for $j > j_L$, the system has a helical SRO with the maximum of $S(q)$ at some $q=Q < \pi$.

In the case of $S=1$, by contrast, no dimer phase occurs [5,6]. The Heisenberg chain is in the Haldane phase characterized by a singlet ground state and a finite en-

ergy gap above it. A first-order transition takes place at $j=j_T \cong 0.744$ between the ‘single-chain’ Haldane phase at $j < j_T$ and the ‘double-chain’ Haldane phase at $j > j_T$ [6]. In the XY case, on the other hand, the situation remains not entirely clear. Analytical studies based on the bosonization method suggested that the gapless phase at $j=0$ (the so-called $XY1$ phase) extended to finite $j > 0$ [7] whereas numerical studies suggested that the Haldane phase was stabilized for $j > 0$ [8]. In any case, the fate of such $XY1$ or Haldane phase at larger j has not been clarified.

In the classical limit $S \rightarrow \infty$, the system exhibits a magnetic LRO, either of the Néel-type ($j \leq 1/4$) or of the helical-type characterized by the wavenumber $q = \cos^{-1}(-1/4j)$ ($j > 1/4$). In the XY case, such helically ordered state possesses a twofold discrete degeneracy according as the helix is either right- or left-handed, in addition to a continuous degeneracy associated with the original $U(1)$ symmetry of the XY spin. This discrete degeneracy is characterized by mutually opposite signs of the total chirality defined by [9]

$$\kappa = \frac{1}{N} \sum_i \kappa_i, \quad (2)$$

$$\kappa_i = S_i^x S_{i+1}^y - S_i^y S_{i+1}^x = [\mathbf{S}_i \times \mathbf{S}_{i+1}]_z,$$

where N is the total number of spins. Chirality is invariant under both $U(1)$ spin-rotation and time-reversal operations, but changes its sign under parity operation. In the Heisenberg case, while there no longer exists a discrete chiral degeneracy, one can still formally define the chirality by Eq.(2) as a z -component of the vector chirality, $\kappa_i = \mathbf{S}_i \times \mathbf{S}_{i+1}$. Note that the chirality defined above is distinct from the scalar chirality of the Heisenberg spin often discussed in the literature [10] defined by $\chi_i = \mathbf{S}_{i-1} \cdot \mathbf{S}_i \times \mathbf{S}_{i+1}$: The scalar chirality of the Heisenberg spin changes sign under the time-reversal operation unlike the chirality (2). Since the classical chain (1) always has a planar spin order, the scalar chirality χ_i vanishes trivially.

Recent studies on various frustrated *classical* systems with continuous symmetry have revealed that such chiral degrees of freedom often give rise to novel ordering behaviors such as phase transitions of new universality class [11], novel magnetic phase diagrams with new multicritical behavior [11], and even a novel ‘chiral phase’ in which only the chirality exhibits a LRO without the standard spin LRO [12–14]. Meanwhile, systematic studies of the possible chiral order in frustrated *quantum* spin chains has been scarce so far.

In this Letter, we perform a numerical study of the ground-state properties of a class of $S=1/2$ and 1 frustrated spin chains (1) in search for a possible chiral order. We have found that both gapless and gapped chiral phases, where the chirality has a finite LRO while the spin correlation falls either algebraically or exponentially, are realized for a wide range of j in the $S=1$ XY chain, but not in the $S=1/2$ XY chain nor in the $S=1/2$ and 1 Heisenberg chains.

In order to probe the possible chiral order, we first calculate the square of the total chirality $\langle \kappa^2 \rangle$, where the chiral order parameter is defined by Eq.(2) now for

quantum spins, together with the associated Binder parameter,

$$g_\kappa = (1 - \frac{\langle \kappa^4 \rangle}{3 \langle \kappa^2 \rangle^2}), \quad (3)$$

by exactly diagonalizing finite open chains with even N up to $N=20$ ($S=1/2$) or $N=16$ ($S=1$) [15]. All ground states are found to belong to the subspace of $S_{\text{total}}^z = 0$ with even parity.

The calculated Binder parameters of the chirality g_κ of the XY chain are shown in Fig.1 for various N as a function of j . As shown in Fig.1(a), g_κ of the $S=1/2$ chain constantly decreases with increasing N for any j , demonstrating the absence of chiral order. In contrast, g_κ of the $S=1$ chain exhibits a significantly different behavior. As can be seen from Fig.1(b), g_κ for various N cross at almost the same j , $j = 0.475 \pm 0.005$, above which g_κ increases with increasing N , indicating the existence of a finite chiral LRO for larger j .

In the case of Heisenberg chains, on the other hand, we have found that for both cases of $S=1/2$ and 1 the calculated g_κ (not shown here) constantly decreases with increasing N , which clearly shows that the chiral order is not realized in the Heisenberg chains.

In order to examine more closely the nature of the transition and of the possible phases, we calculate, concentrating on the $S=1$ XY open chain, the two-point chiral, spin, and string correlation functions defined by

$$C_\kappa(r) = \langle \kappa_{r_0-r/2} \kappa_{r_0+r/2} \rangle, \quad (4)$$

$$C_s(r) = \langle S_{r_0-r/2}^x S_{r_0+r/2}^x \rangle, \quad (5)$$

$$C_{\text{str}}(r) = \langle S_{r_0-r/2}^z (\exp i\pi \sum_{j=r_0-r/2+1}^{r_0+r/2-1} S_j^z) S_{r_0+r/2}^z \rangle, \quad (6)$$

by means of the density-matrix renormalization-group method. [16]. Here r_0 represents the center position of open chain, *i.e.*, $r_0=N/2$ for even r and $r_0=(N+1)/2$ for odd r . We employ the infinite system method by using M block states ($M \leq 300$) in the subspace of $S_{\text{total}}^z=0$ with even parity. Convergence of the results with respect to M has been checked by consecutively increasing M . In the chiral phase, the chiral correlation function $C_\kappa(r)$ tends to a finite constant at large r , while in the Haldane phase, the string correlation function $C_{\text{str}}(r)$ tends to a finite constant.

The calculated r -dependence of the chiral, string, and spin correlation functions are shown in Fig.2(a)-(c) on log-log plots for several typical values of j . As can be seen from Fig.2(a), the data of $C_\kappa(r)$ for $j > j_{c1} \simeq 0.473$ bend up at larger r suggesting a finite chiral LRO, while they bend down for $j < j_{c1}$ suggesting the absence of chiral order. Our estimate of $j_{c1} = 0.473 \pm 0.001$ is consistent with the estimate from the Binder parameter given above. Meanwhile, as shown in Fig.2(b), the data of

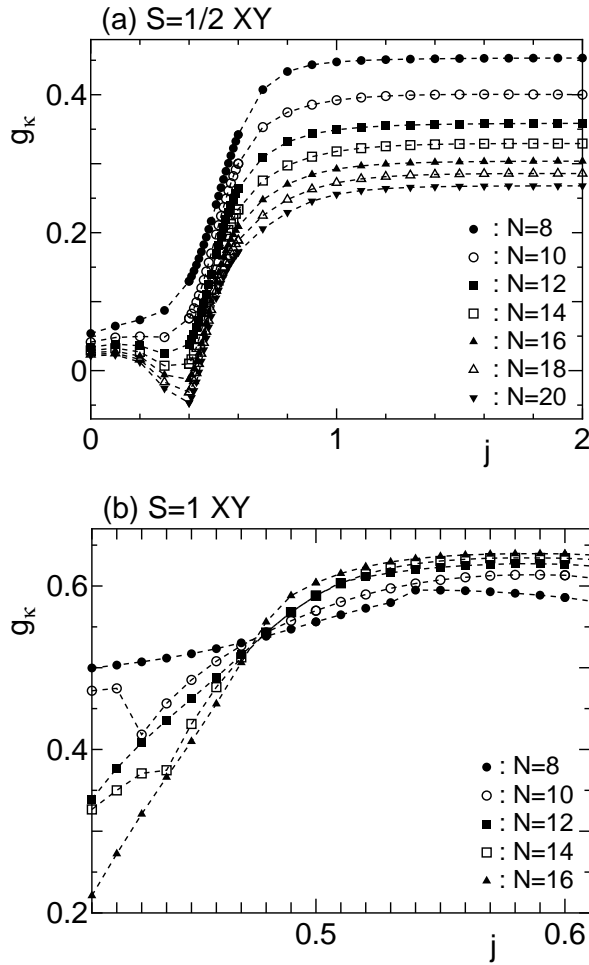


FIG. 1. Binder parameter of the chirality g_κ versus j : (a) $S=1/2$ XY chain; (b) $S=1$ XY chain.

$C_{str}(r)$ for $j < j_{c2} \simeq 0.490$ bend up for larger r suggesting a finite string order characteristic of the Haldane state, while for $j > j_{c2}$ they show a linear behavior signaling a power-law decay of the string correlation. The existence of the Haldane phase for smaller j is consistent with the previous finding of Ref. [8].

An interesting observation here is that our estimate of $j_{c2} = 0.490^{+0.010}_{-0.005}$ is distinctly larger than that of $j_{c1} = 0.473 \pm 0.001$, which means that *there exist two different types of chiral phases*, one with a finite string order ($j_{c1} < j < j_{c2}$) and the other without the string order ($j > j_{c2}$). This finding is also supported by the behavior of the spin correlation function $C_s(r)$ in Fig.2(c), in which $C_s(r)$ divided by the oscillating factor $\cos(Qr)$ is shown. Indeed, the data of $C_s(r)$ exhibit a linear behavior for $j > j_{c2}$ indicating a power-law decay of helical spin correlations (gapless state), while for $j < j_{c2}$ they bend down suggesting an exponential-decay of helical spin correlations (gapped state). Note that above the Lifshitz point, which we estimate to be $j_L = 0.313 \pm 0.001$ for the $S = 1$ XY chain, the system exhibits a helical SRO characterized by a wavevector $Q < \pi$. On the other hand, the absence of magnetic (spin) LRO has rigorously been proven for any j and for general $S < \infty$ [17]. The existence of a novel intermediate phase, a gapped chiral phase, in a narrow but finite range of j can clearly be seen in Fig.2 from the behavior of the correlation functions at $j = 0.477$ which lies between j_{c1} and j_{c2} .

Thus, on increasing j , the $S = 1$ XY spin chain undergoes two successive transitions, first at $j = j_{c1}$ from the Haldane phase with no chiral order to the gapped chiral phase (or the chiral Haldane phase), then at $j = j_{c2}$ from the gapped chiral phase to the gapless chiral phase. In the gapped chiral phase, the chiral and string LRO coexist with exponentially-decaying spin correlations, whereas in the gapless chiral phase, only the chirality shows a LRO with algebraically-decaying spin and string correlations. In the gapped (gapless) chiral phase, the ground state is doubly degenerate, each of which is characterized by the opposite sense of the chirality, with (without) a finite gap above it.

The gapped chiral phase is characterized by a spontaneously broken parity with preserving both translation and time-reversal symmetries. From a broken symmetry, the transition at $j = j_{c1}$ is expected to be of the Ising-type. We extract the chiral correlation length ξ_κ from the calculated $C_\kappa(r)$ and fit it to the standard power-law form $\xi_\kappa \sim (j_{c1} - j)^{-\nu_\kappa}$. Our present estimate, $\nu_\kappa \simeq 0.9 \pm 0.1$ appears to be slightly smaller than, but not inconsistent with the 2D Ising value $\nu_\kappa = 1$. Further detailed study of the critical properties, including the nature of the KT-like transition at $j = j_{c2}$, is in progress.

It should be noticed that Nersesyan *et al.* recently discussed for the $S=1/2$ XY chain in the limit of large j the possibility of the parity breaking [18]. In contrast to this suggestion, for the $S=1/2$ XY and Heisenberg

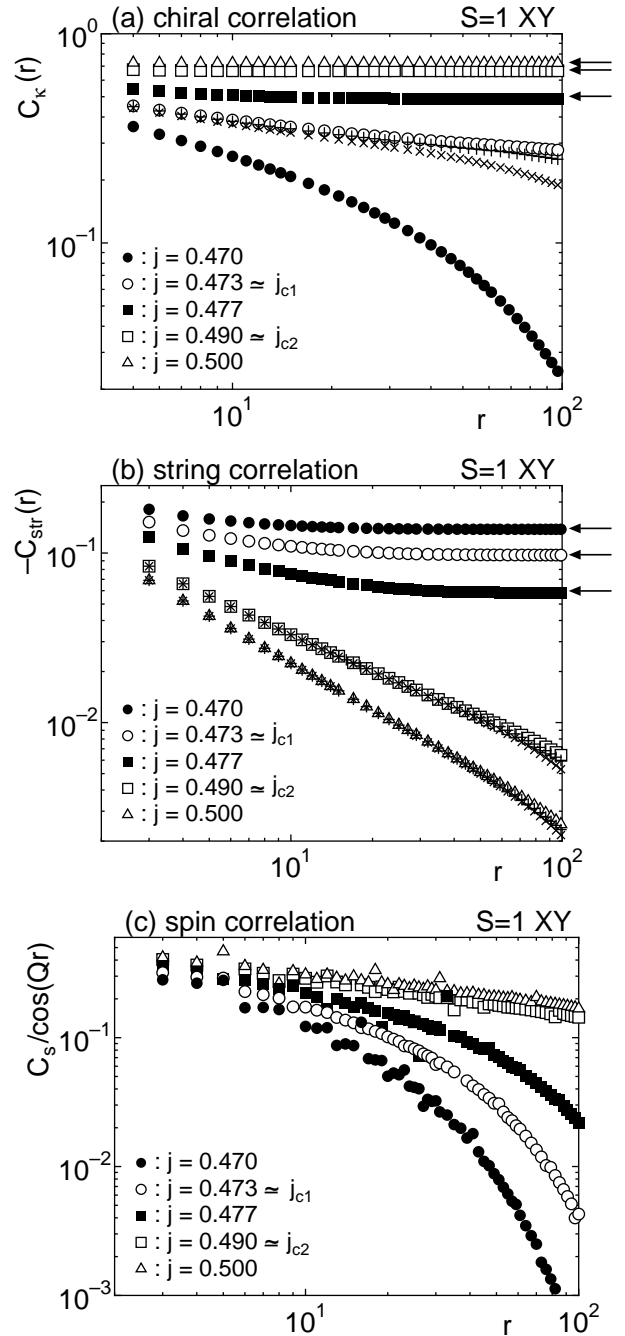


FIG. 2. Correlation functions versus r on log-log plots for various j : (a) chiral correlation $C_\kappa(r)$; (b) string correlation $-C_{str}(r)$; (c) spin correlation $C_s(r)$ divided by the oscillating factor $\cos(Qr)$. Arrows in the figures represent the extrapolated $r = \infty$ values. The number of block states is equal to $M = 300$. To illustrate the M -dependence, we also indicate by crosses the data for $M = 220$ and 260 for several cases where the M -dependence is relative large. Note that some of the data points for larger r are omitted for clarity.

chains, we did not find the chiral phase [19] nor any new phase except for the well-known spin-fluid and dimer phases, corroborating the type of the phase diagram previously reported by Haldane [4] and by Tonegawa *et al*

[1]. The chiral phase found here appears to be specific to the $S = 1$ XY chain. Such tendency may roughly be understood by noting that only the XY chain sustains an Ising-like discrete chirality which has a stronger ordering tendency than the continuous spin variable while quantum fluctuations might be strong enough in the $S = 1/2$ chain to wash out even the chiral ordering.

It might also be interesting to notice that the observed novel transition behavior of the $S = 1$ XY chain has a similarity to that of the 2D frustrated classical XY models such as the triangular-lattice XY antiferromagnet [12] or the Josephson-junction array in a magnetic field [13]. In these classical systems, Miyashita and Shiba, and more recently Olsson observed by Monte Carlo simulations that the thermal phase transitions occurred in two steps with two types of chiral phases, each characterized by exponentially-decaying and algebraically-decaying spin correlations. At the moment, we donot know whether there exists a deeper connection between the two systems.

Finally, we wish to briefly discuss the possible experimental implication of our results. In order to observe the chiral phase, one needs to prepare an $S = 1$ XY zig-zag chain with its j value in a suitable range. In the presence of weak 3D interchain interaction, while the gapless chiral phase stabilized for larger j is expected to show the standard helical spin LRO, the gapped chiral phase could remain gapped. Hence, it is challenging to experimentally observe the gapped chiral state in an appropriate model material. One problem here might be that the gapped chiral phase is realized in a rather narrow range of j . It might then be necessary to tune the j value by some experimental method, such as by applying pressure. Once an appropriate sample could be prepared, it is in principle possible to measure the chirality by using, *e.g.*, polarized neutrons. [11,20]

In summary, from numerical studies of the ground-state properties of a class of $S=1/2$ and 1 frustrated spin chains we have found that both gapless and gapped chiral phases, where the chirality has a finite LRO while the spin correlation falls either algebraically or exponentially, are realized for a wide range of j in the $S=1$ XY chain, but not in the $S=1/2$ XY chain nor in the $S=1/2$ and 1 Heisenberg chains. Further details of the results including the critical properties and the full phase diagrams will be reported elsewhere.

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